Full wwPDB X-ray Structure Validation Report (i)

May 23, 2024 – 10:38 AM EDT

PDB ID	:	3ZHT
Title	:	Crystal structure of the SucA domain of Mycobacterium smegmatis KGD, first post-decarboxylation intermediate from 2-oxoadipate
Authors	:	Wagner, T.; Barilone, N.; Bellinzoni, M.; Alzari, P.M.
Deposited on	:	2012-12-24
Resolution	:	2.15 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

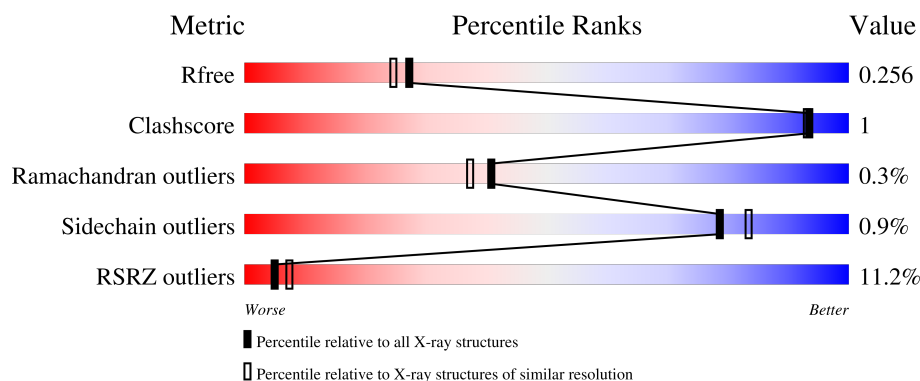|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.256
Clashscore		1
Ramachandran outliers		0.3%
Sidechain outliers		0.9%
RSRZ outliers		11.2%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	868	10% / 88% / 5% 6%
1	B	868	11% / 89% / · 7%
1	C	868	9% / 89% / · 7%
1	D	868	12% / 89% / · 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 26205 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	814	Total	C	N	O	S	0	1	0
			6292	3963	1111	1194	24			
1	B	809	Total	C	N	O	S	0	2	0
			6224	3922	1101	1176	25			
1	C	808	Total	C	N	O	S	0	0	0
			6258	3940	1104	1191	23			
1	D	807	Total	C	N	O	S	0	0	0
			6199	3905	1091	1180	23			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	360	GLY	-	expression tag	UNP A0R2B1
B	360	GLY	-	expression tag	UNP A0R2B1
C	360	GLY	-	expression tag	UNP A0R2B1
D	360	GLY	-	expression tag	UNP A0R2B1

- Molecule 2 is (5S)-5-{3-[(4-amino-2-methylpyrimidin-5-yl)methyl]-4-methyl-5-(2-{[(phospho natooxy)phosphinato]oxy}ethyl)-1,3-thiazol-3-ium-2-yl}-5-hydroxypentanoate (three-letter code: TD9) (formula: $C_{17}H_{27}N_4O_{10}P_2S$).
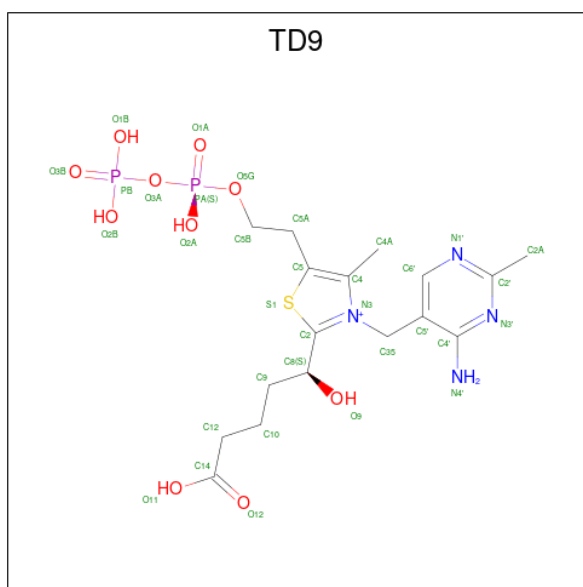
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			34	17	4	10	2	1		
2	B	1	Total	C	N	O	P	S	0	0
			34	17	4	10	2	1		
2	C	1	Total	C	N	O	P	S	0	0
			34	17	4	10	2	1		
2	D	1	Total	C	N	O	P	S	0	0
			34	17	4	10	2	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Ca 1	0	0
4	C	1	Total 1	Ca 1	0	0
4	D	1	Total 1	Ca 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	339	Total 339	O 339	0	0
5	B	223	Total 223	O 223	0	0
5	C	305	Total 305	O 305	0	0
5	D	221	Total 221	O 221	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in 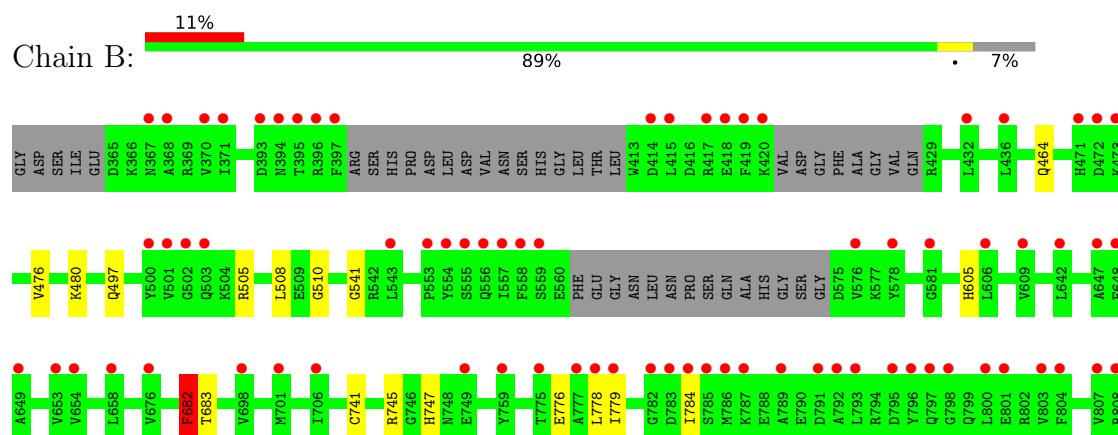geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

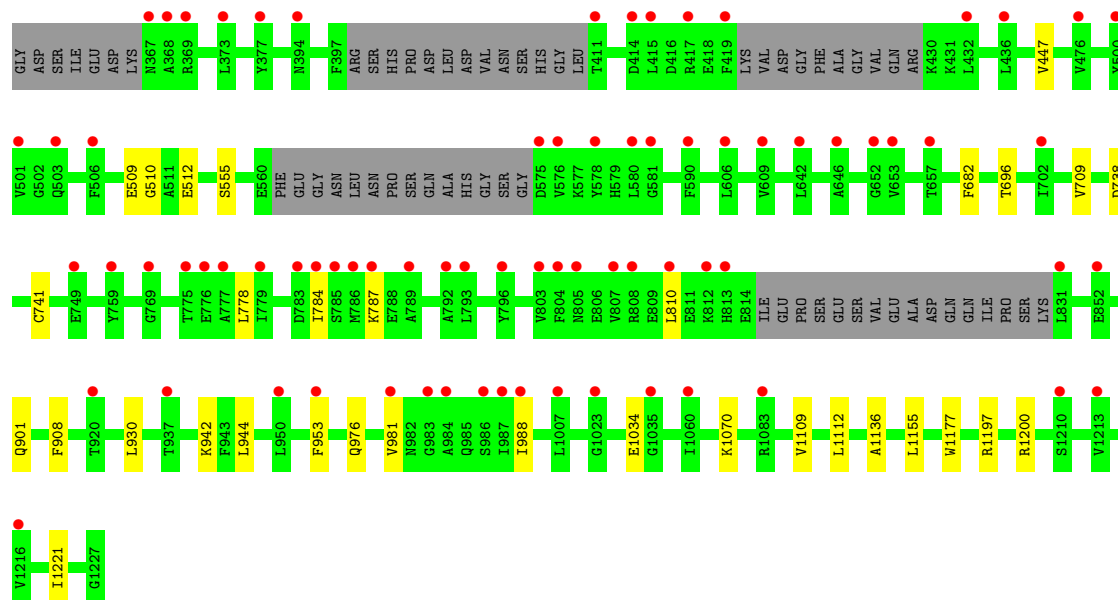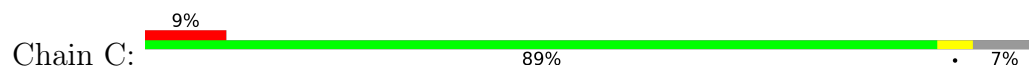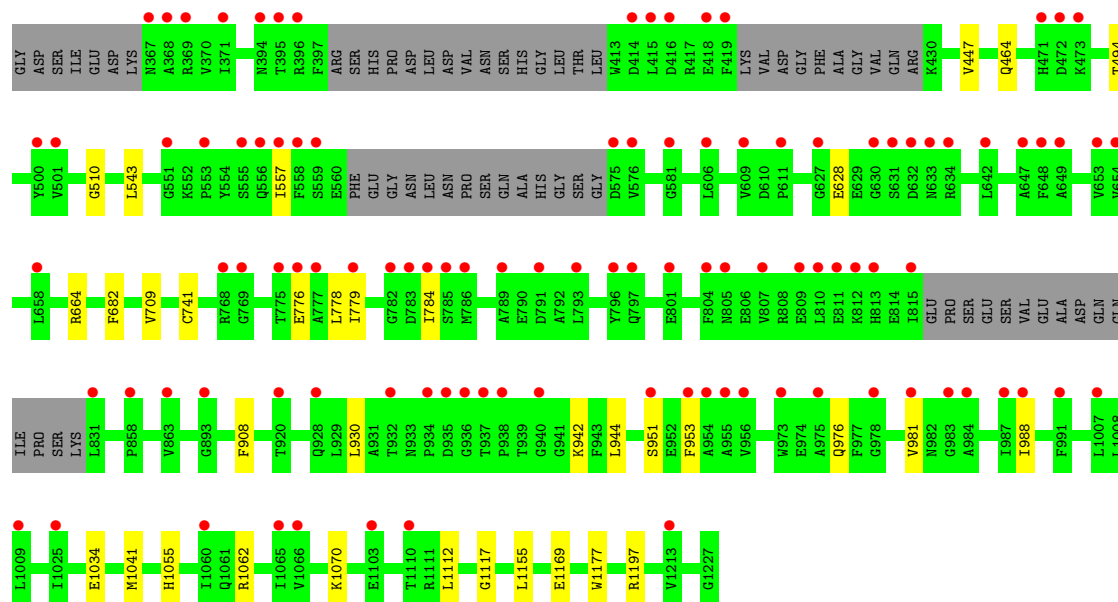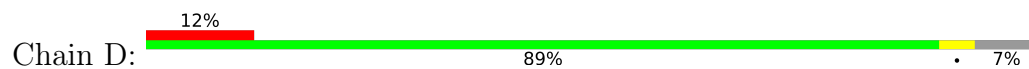E809 L810 E811 K812 H813 GLU ILE GLU PRO SER GLU SER VAL GLU ALA ASP GLN GLN ILE PRO SER LYS L831 D836 R842 P858 F908 V916 Q928 L929 L930 A931 T932 P938 T939 G940 F953 A954 Q976 F977 G978 V981 N982 G983 A984 I987 I988 I1025

E1034 G1035 H1055 R1062 K1070 E1103 L1112 L1155 W1177 R1197 R1200 V1213 I1221 A1225 F1226 G1227

● Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

Chain C:

9%
89% 7%

GLY ASP SER ILE GLU ASP LYS N367 A368 R369 L373 Y377 N394 F397 ARG SER HIS PRO ASP LEU ASP VAL ASN SER HIS GLY LEU T411 D414 L415 D416 R417 E418 F419 LYS VAL ASP GLY PHE ALA GLY VAL GLN ARG K430 K431 L432 L436 V447 V476 Y500

V501 G502 Q503 E506 E509 G510 A511 E512 S555 E560 PHE GLU GLY ASN LEU ASN PRO SER GLN ALA HIS GLY SER GLY D575 V576 K577 Y578 H579 L580 G581 F590 L606 V609 L642 A646 G652 V653 T657 F682 T696 I702 V709 D738

C741 E749 Y759 G769 T775 E776 A777 L778 I779 D783 I784 S785 M786 K787 E788 A789 A792 L793 Y796 V803 F804 N805 E806 V807 R808 E809 L810 E811 K812 H813 E814 ILE GLU PRO SER GLU SER VAL GLU ALA ASP GLN GLN ILE PRO SER LYS L831 E852

Q901 F908 T920 L930 T937 K942 F943 L944 L950 F953 Q976 V981 N982 G983 A984 Q985 S986 I987 I988 L1007 G1023 E1034 G1035 I1060 K1070 R1083 V1109 L1112 A1136 L1155 W1177 R1197 R1200 S1210 V1213

V1216 I1221 G1227

● Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

Chain D:

12%
89% 7%

GLY ASP SER ILE GLU ASP LYS N367 A368 R369 V370 I371 N394 T395 R396 F397 ARG SER HIS PRO ASP LEU ASP VAL ASN SER HIS GLY LEU THR LEU W413 D414 L415 D416 R417 E418 F419 LYS VAL ASP GLY PHE ALA GLY VAL GLN ARG K430 V447 Q464 H471 D472 K473 T494

Y500 V501 G510 L543 G551 K552 P553 Y554 S555 Q556 I557 F558 S559 E560 PHE GLU GLY ASN LEU ASN PRO SER GLN ALA HIS GLY SER GLY D575 V576 G581 L606 V609 D610 P611 G627 E628 E629 G630 S631 D632 N633 R634 L642 A647 F648 A649 V653 V654

L658 R664 F682 V709 C741 R768 G769 T775 E776 A777 L778 I779 G782 D783 I784 S785 M786 A789 E790 D791 A792 L793 Y796 Q797 E801 F804 N805 E806 V807 R808 E809 L810 E811 K812 H813 E814 I815 GLU PRO SER GLU SER VAL GLU ALA ASP GLN GLN

ILE PRO SER LYS L831 P858 V863 G893 F908 T920 Q928 L929 L930 A931 T932 N933 P934 D935 G936 T937 P938 T939 G940 G941 K942 F943 L944 S951 E952 F953 A954 A955 V956 W973 E974 A975 Q976 F977 G978 V981 N982 G983 A984 I987 I988 F991 L1007 L1008

L1009 I1025 E1034 M1041 H1055 I1060 Q1061 R1062 I1065 V1066 K1070 E1103 T1110 R1111 L1112 G1117 L1155 E1169 W1177 R1197 V1213 G1227

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	80.37Å 83.80Å 159.51Å 99.76° 99.06° 100.61°	Depositor
Resolution (Å)	41.11 – 2.15 41.11 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.5 (41.11-2.15) 97.5 (41.11-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.16Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.223 , 0.246 0.228 , 0.256	Depositor DCC
R_{free} test set	10531 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 55.9	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	26205	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.1817e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TD9, MG, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.50	0/6422	0.62	0/8710
1	B	0.48	0/6356	0.62	0/8627
1	C	0.50	0/6384	0.61	0/8657
1	D	0.48	0/6324	0.62	0/8584
All	All	0.49	0/25486	0.62	0/34578

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6292	0	6064	23	0
1	B	6224	0	5986	18	0
1	C	6258	0	6043	15	0
1	D	6199	0	5953	15	0
2	A	34	0	23	0	0
2	B	34	0	23	1	0
2	C	34	0	23	0	0
2	D	34	0	23	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	339	0	0	0	0
5	B	223	0	0	1	0
5	C	305	0	0	0	0
5	D	221	0	0	1	0
All	All	26205	0	24138	71	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (71) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1035:GLY:O	1:B:1062:ARG:HD2	1.90	0.71
1:D:1112:LEU:HD21	1:D:1155:LEU:HD22	1.84	0.59
1:B:497:GLN:HG3	1:B:745:ARG:HH12	1.68	0.59
1:B:1112:LEU:HD21	1:B:1155:LEU:HD22	1.85	0.57
1:C:1112:LEU:HD21	1:C:1155:LEU:HD22	1.87	0.56
1:B:476:VAL:HG12	1:B:480:LYS:HE2	1.87	0.55
1:A:544:ASN:OD1	1:A:548:ASN:ND2	2.41	0.54
1:C:509:GLU:HA	1:C:512:GLU:OE2	2.09	0.53
1:D:942:LYS:HE2	1:D:944:LEU:HD21	1.90	0.53
1:B:497:GLN:HG3	1:B:745:ARG:NH1	2.26	0.51
1:A:555:SER:HA	1:A:810:LEU:HD22	1.92	0.51
1:C:981:VAL:HG22	1:C:988:ILE:HD11	1.93	0.51
1:D:981:VAL:HG22	1:D:988:ILE:HD11	1.92	0.51
1:A:843:ILE:HG12	1:A:930:LEU:HD21	1.94	0.50
1:A:981:VAL:HG22	1:A:988:ILE:HD11	1.93	0.50
1:B:505:ARG:HA	1:B:747:HIS:O	2.12	0.49
1:B:981:VAL:HG22	1:B:988:ILE:HD11	1.94	0.49
1:A:744:ARG:HG3	1:A:745:ARG:HG3	1.96	0.48
1:D:1041:MET:HE2	1:D:1117:GLY:HA3	1.96	0.48
1:B:908:PHE:CZ	1:B:1070:LYS:HG2	2.49	0.47
1:B:778:LEU:HB3	1:B:784:ILE:HG12	1.95	0.47
1:A:901:GLN:OE1	2:B:2001:TD9:H6'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:ARG:HA	1:A:747:HIS:O	2.15	0.47
1:A:778:LEU:HB3	1:A:784:ILE:HG12	1.97	0.46
1:A:561:PHE:O	1:A:562:GLU:HB2	2.16	0.46
1:C:555:SER:HA	1:C:810:LEU:HD22	1.98	0.46
1:A:908:PHE:CZ	1:A:1070:LYS:HG2	2.51	0.46
1:C:1177:TRP:CD1	1:C:1197:ARG:HD3	2.52	0.45
1:D:1169:GLU:OE1	5:D:3208:HOH:O	2.21	0.45
1:C:510:GLY:O	1:C:741:CYS:HB2	2.17	0.45
1:C:908:PHE:CZ	1:C:1070:LYS:HG2	2.52	0.45
1:A:492:PHE:CE1	1:A:496:LEU:HD13	2.53	0.44
1:D:776:GLU:HA	1:D:779:ILE:HD12	1.99	0.44
1:C:1112:LEU:CD2	1:C:1155:LEU:HD22	2.48	0.44
1:A:843:ILE:HG12	1:A:930:LEU:CD2	2.47	0.44
1:D:908:PHE:CZ	1:D:1070:LYS:HG2	2.53	0.44
1:A:510:GLY:O	1:A:741:CYS:HB2	2.18	0.43
1:B:776:GLU:HA	1:B:779:ILE:HD12	1.98	0.43
1:A:843:ILE:CG1	1:A:930:LEU:HD21	2.48	0.43
1:B:1055:HIS:HE1	1:B:1062:ARG:O	2.01	0.43
1:B:510:GLY:O	1:B:741:CYS:HB2	2.18	0.43
1:D:510:GLY:O	1:D:741:CYS:HB2	2.18	0.43
1:A:1177:TRP:CD1	1:A:1197:ARG:HD3	2.53	0.43
1:D:1177:TRP:CD1	1:D:1197:ARG:HD3	2.54	0.43
1:D:628:GLU:HG2	1:D:664:ARG:O	2.19	0.42
1:B:682:PHE:CD1	1:B:683:THR:HG23	2.54	0.42
1:A:509:GLU:HA	1:A:512:GLU:OE2	2.20	0.42
1:C:1109:VAL:HG21	1:C:1136:ALA:HB2	2.00	0.42
1:D:778:LEU:HB3	1:D:784:ILE:HG12	2.01	0.42
1:B:1177:TRP:CD1	1:B:1197:ARG:HD3	2.54	0.42
1:D:1055:HIS:HE1	1:D:1062:ARG:O	2.03	0.42
1:A:628:GLU:HG2	1:A:664:ARG:O	2.20	0.41
1:D:543:LEU:HD22	1:D:557:ILE:HG23	2.01	0.41
1:C:447:VAL:HG22	1:C:709:VAL:HG12	2.01	0.41
1:C:778:LEU:HB3	1:C:784:ILE:HG12	2.02	0.41
1:A:903:THR:O	1:A:911:ARG:HD2	2.21	0.41
1:D:447:VAL:HG22	1:D:709:VAL:HG12	2.02	0.41
1:B:842:ARG:NH2	1:B:932:THR:O	2.53	0.41
1:D:1112:LEU:CD2	1:D:1155:LEU:HD22	2.50	0.41
1:A:696:THR:HG21	1:A:738:ASP:HB2	2.02	0.41
1:A:1200:ARG:HG3	1:A:1221:ILE:HD11	2.03	0.41
1:B:1200:ARG:HG3	1:B:1221:ILE:HD11	2.03	0.41
1:A:842:ARG:NH2	1:A:932:THR:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1200:ARG:HG3	1:C:1221:ILE:HD11	2.02	0.41
1:A:1055:HIS:HE1	1:A:1062:ARG:O	2.03	0.40
1:B:508:LEU:HD13	1:B:541:GLY:HA3	2.03	0.40
1:B:747:HIS:HA	5:B:3035:HOH:O	2.21	0.40
1:A:942:LYS:HE3	1:A:944:LEU:HD21	2.03	0.40
1:C:696:THR:HG21	1:C:738:ASP:HB2	2.03	0.40
1:C:901:GLN:OE1	2:D:2001:TD9:H6'	2.21	0.40
1:C:942:LYS:HE3	1:C:944:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	805/868 (93%)	784 (97%)	18 (2%)	3 (0%)	34	29
1	B	801/868 (92%)	780 (97%)	18 (2%)	3 (0%)	34	29
1	C	798/868 (92%)	776 (97%)	21 (3%)	1 (0%)	51	53
1	D	797/868 (92%)	778 (98%)	18 (2%)	1 (0%)	51	53
All	All	3201/3472 (92%)	3118 (97%)	75 (2%)	8 (0%)	41	46

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	561	PHE
1	B	1034	GLU
1	D	1034	GLU
1	A	1034	GLU
1	C	1034	GLU
1	A	605	HIS
1	B	605	HIS

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Mol	Chain	Res	Type
1	B	682	PHE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	646/726 (89%)	641 (99%)	5 (1%)	81	86
1	B	635/726 (88%)	630 (99%)	5 (1%)	81	86
1	C	645/726 (89%)	640 (99%)	5 (1%)	81	86
1	D	633/726 (87%)	626 (99%)	7 (1%)	73	78
All	All	2559/2904 (88%)	2537 (99%)	22 (1%)	78	83

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	496	LEU
1	A	682	PHE
1	A	953	PHE
1	A	976	GLN
1	A	1112	LEU
1	B	464	GLN
1	B	682	PHE
1	B	930	LEU
1	B	953	PHE
1	B	976	GLN
1	C	682	PHE
1	C	787	LYS
1	C	930	LEU
1	C	953	PHE
1	C	976	GLN
1	D	464	GLN
1	D	494	THR
1	D	682	PHE
1	D	930	LEU
1	D	951	SER

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Mol	Chain	Res	Type
1	D	953	PHE
1	D	976	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	TD9	A	2001	3	30,35,35	1.37	2 (6%)	36,51,51	1.52	4 (11%)
2	TD9	B	2001	3	30,35,35	1.30	3 (10%)	36,51,51	1.36	4 (11%)
2	TD9	D	2001	3	30,35,35	1.63	3 (10%)	36,51,51	1.36	4 (11%)
2	TD9	C	2001	3	30,35,35	1.41	3 (10%)	36,51,51	1.50	4 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TD9	A	2001	3	-	4/22/27/27	0/2/2/2
2	TD9	B	2001	3	-	6/22/27/27	0/2/2/2
2	TD9	D	2001	3	-	7/22/27/27	0/2/2/2
2	TD9	C	2001	3	-	4/22/27/27	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2001	TD9	C5-S1	-5.37	1.64	1.74
2	A	2001	TD9	C2-N3	5.28	1.47	1.35
2	D	2001	TD9	C5A-C5	5.25	1.53	1.50
2	A	2001	TD9	C5-S1	-4.97	1.64	1.74
2	D	2001	TD9	C2-N3	4.97	1.46	1.35
2	B	2001	TD9	C2-N3	4.85	1.46	1.35
2	C	2001	TD9	C2-N3	4.67	1.45	1.35
2	B	2001	TD9	C5-S1	-4.14	1.66	1.74
2	D	2001	TD9	C5-S1	-4.09	1.66	1.74
2	C	2001	TD9	C5A-C5	2.18	1.51	1.50
2	B	2001	TD9	C5A-C5	2.12	1.51	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2001	TD9	PA-O3A-PB	6.69	155.78	132.83
2	A	2001	TD9	PA-O3A-PB	6.52	155.20	132.83
2	D	2001	TD9	PA-O3A-PB	6.05	153.59	132.83
2	B	2001	TD9	PA-O3A-PB	5.80	152.72	132.83
2	A	2001	TD9	O1B-PB-O3A	-3.33	93.46	104.64
2	C	2001	TD9	O1B-PB-O3A	-3.08	94.30	104.64
2	D	2001	TD9	O1B-PB-O3A	-2.63	95.80	104.64
2	A	2001	TD9	C5A-C5-C4	-2.51	125.42	127.43
2	D	2001	TD9	C5-C4-N3	2.32	112.52	107.66
2	A	2001	TD9	C5-C4-N3	2.30	112.48	107.66
2	B	2001	TD9	O2B-PB-O3B	2.26	119.54	110.68
2	B	2001	TD9	C5-C4-N3	2.13	112.12	107.66
2	C	2001	TD9	C5A-C5-C4	-2.11	125.74	127.43
2	B	2001	TD9	O1B-PB-O3A	-2.09	97.63	104.64
2	D	2001	TD9	O5G-PA-O1A	2.07	117.17	109.07
2	C	2001	TD9	C5-C4-N3	2.07	111.98	107.66

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2001	TD9	C2-C8-C9-C10
2	B	2001	TD9	O9-C8-C9-C10
2	C	2001	TD9	PB-O3A-PA-O5G
2	D	2001	TD9	O9-C8-C9-C10
2	D	2001	TD9	N3-C35-C5'-C4'
2	D	2001	TD9	C9-C10-C12-C14
2	A	2001	TD9	PB-O3A-PA-O5G
2	B	2001	TD9	PB-O3A-PA-O5G
2	D	2001	TD9	PB-O3A-PA-O5G
2	D	2001	TD9	C12-C10-C9-C8
2	A	2001	TD9	C10-C12-C14-O12
2	C	2001	TD9	C10-C12-C14-O12
2	A	2001	TD9	C10-C12-C14-O11
2	C	2001	TD9	C10-C12-C14-O11
2	A	2001	TD9	C12-C10-C9-C8
2	C	2001	TD9	C12-C10-C9-C8
2	B	2001	TD9	C10-C12-C14-O11
2	B	2001	TD9	PA-O3A-PB-O2B
2	D	2001	TD9	PA-O3A-PB-O2B
2	B	2001	TD9	C10-C12-C14-O12
2	D	2001	TD9	C5B-O5G-PA-O1A

There are no ring outliers.
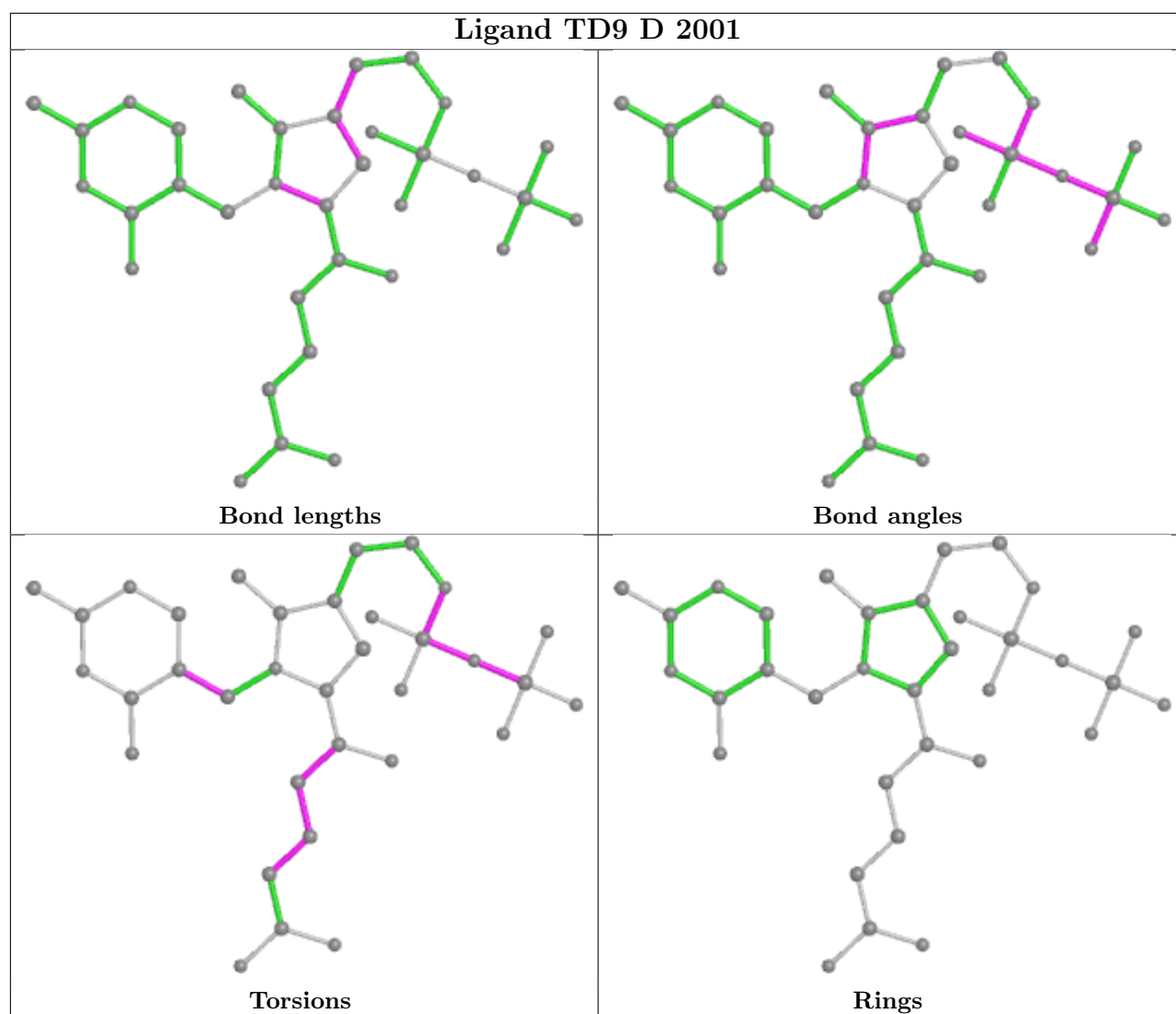
2 monomers are involved in 2 short contacts:

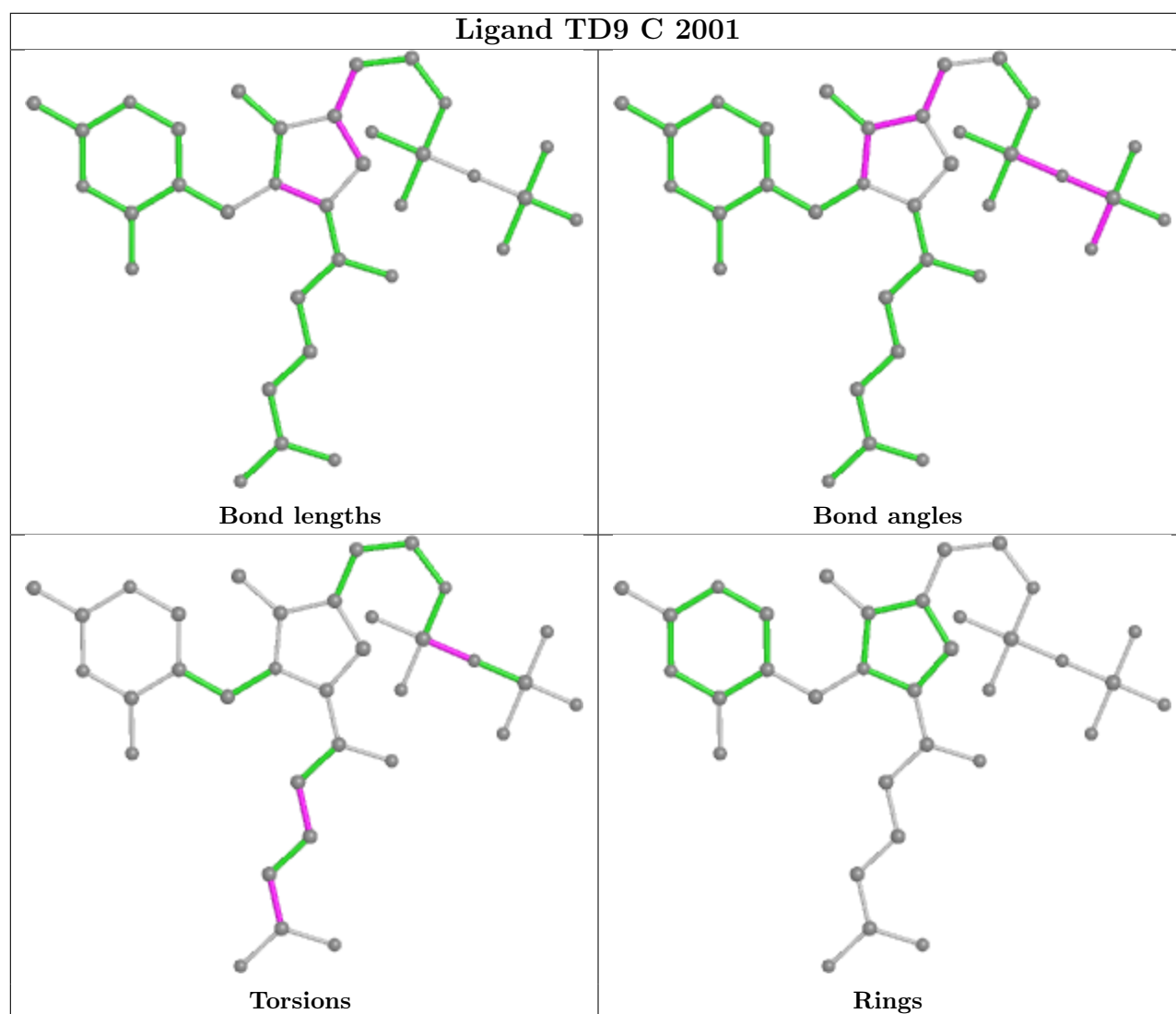| Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	TD9	1	0
2	D	2001	TD9	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.

Ligand TD9 A 2001	
Bond lengths	Bond angles
Torsions	Rings

Ligand TD9 B 2001

Bond lengths

Bond angles

Torsions

Rings

Full wwPDB X-ray Structure Validation Report

Ligand TD9 D 2001

Bond lengths

Bond angles

Torsions

Rings

Ligand TD9 C 2001
Bond lengths · Bond angles · Torsions · Rings
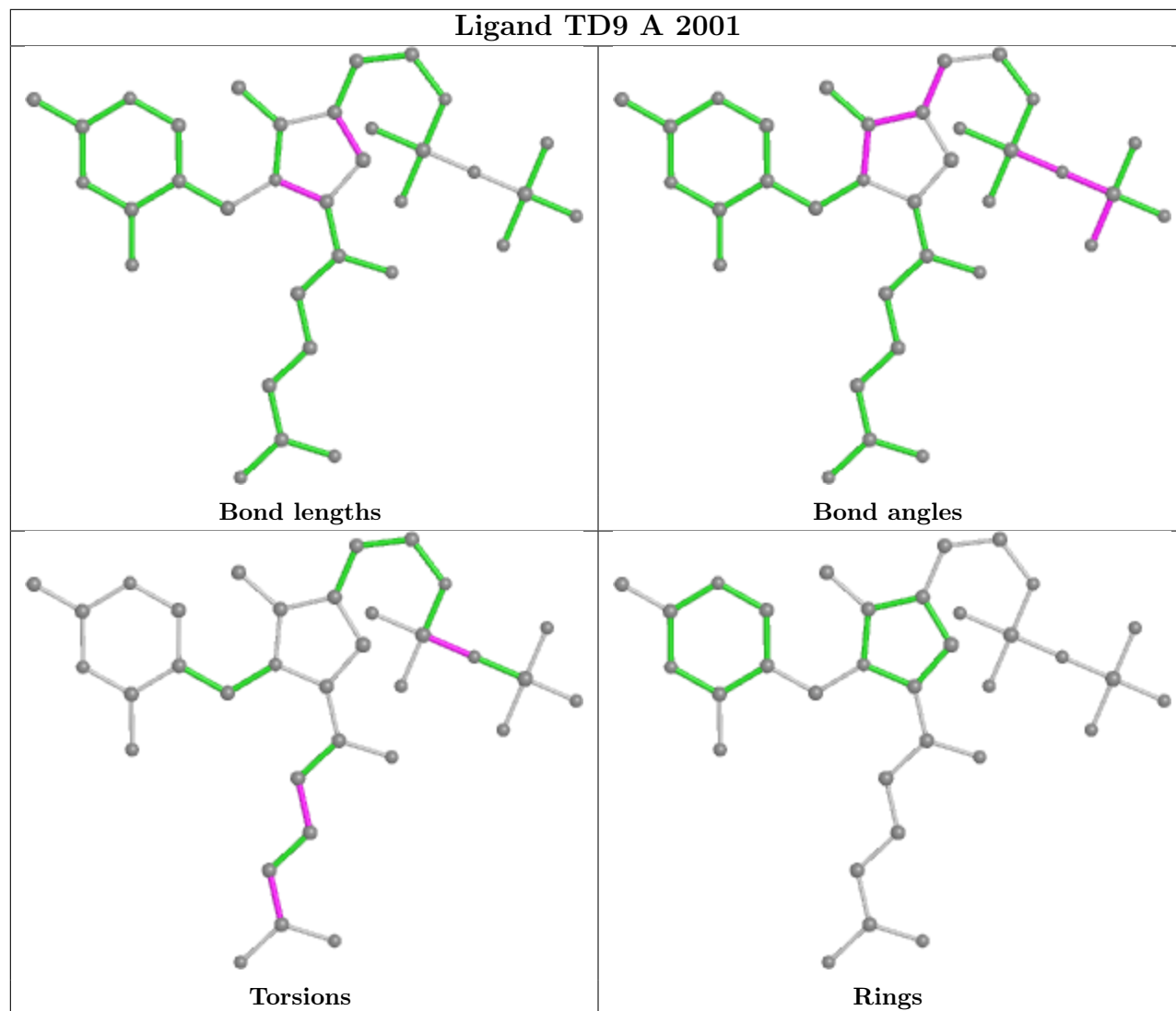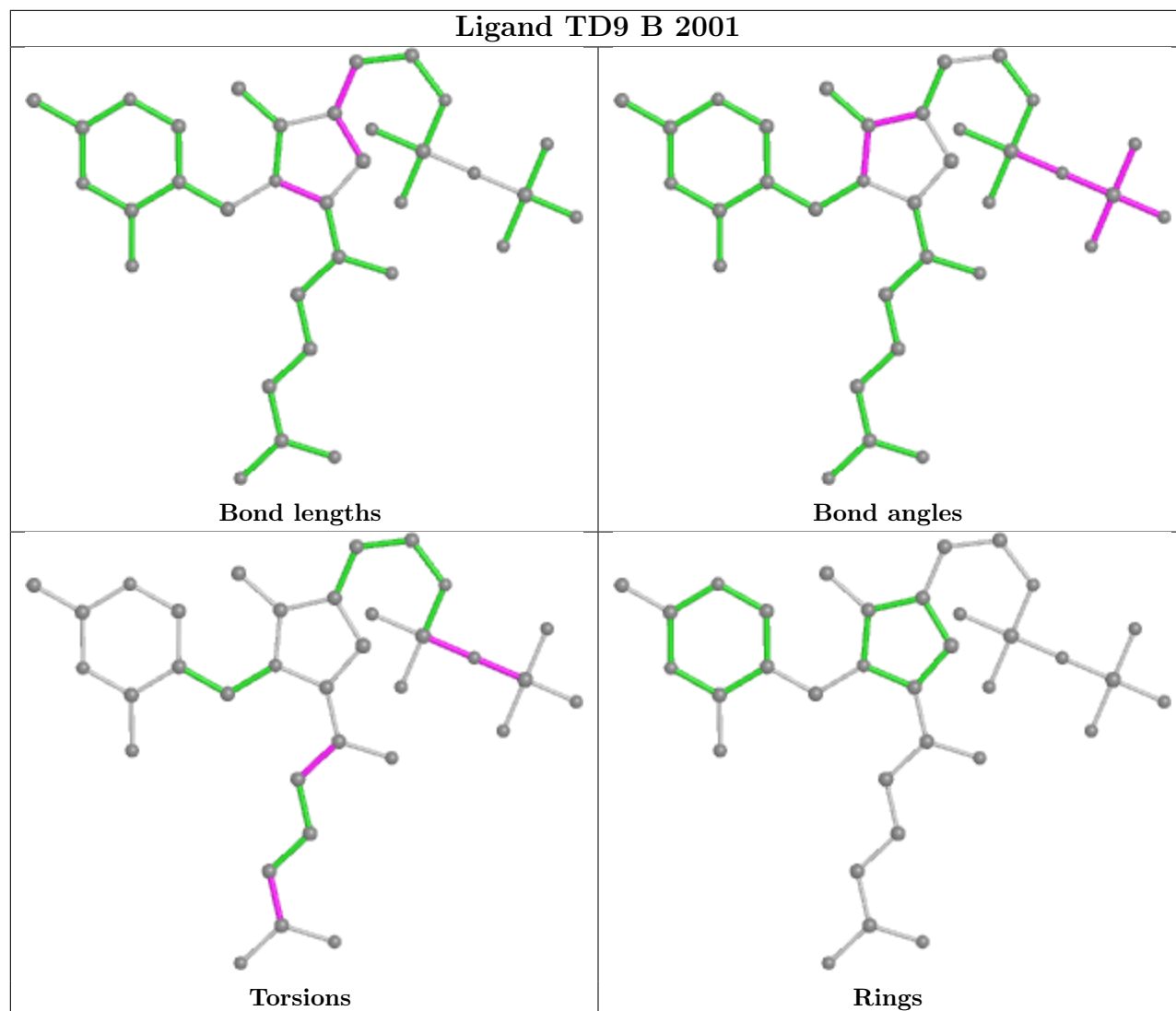
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	814/868 (93%)	0.55	86 (10%)	6	9	23, 39, 71, 113	0
1	B	809/868 (93%)	0.67	97 (11%)	4	6	24, 43, 76, 111	0
1	C	808/868 (93%)	0.52	76 (9%)	8	12	23, 39, 70, 97	0
1	D	807/868 (92%)	0.70	105 (13%)	3	4	23, 42, 76, 104	0
All	All	3238/3472 (93%)	0.61	364 (11%)	5	7	23, 41, 74, 113	0

All (364) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	501	VAL	13.1
1	D	501	VAL	11.2
1	A	368	ALA	8.4
1	D	368	ALA	8.3
1	B	368	ALA	8.1
1	B	367	ASN	8.0
1	D	810	LEU	7.3
1	B	810	LEU	7.2
1	C	779	ILE	7.0
1	B	777	ALA	7.0
1	A	561	PHE	7.0
1	B	807	VAL	6.3
1	B	419	PHE	6.2
1	C	810	LEU	6.1
1	B	394	ASN	6.0
1	B	793	LEU	5.9
1	C	368	ALA	5.8
1	C	769	GLY	5.7
1	C	785	SER	5.7
1	D	785	SER	5.6
1	C	419	PHE	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	785	SER	5.2
1	C	415	LEU	5.1
1	D	395	THR	5.1
1	D	419	PHE	5.0
1	D	779	ILE	5.0
1	C	394	ASN	5.0
1	A	1210	SER	4.9
1	D	793	LEU	4.9
1	B	500	TYR	4.9
1	C	369	ARG	4.9
1	B	779	ILE	4.9
1	D	813	HIS	4.8
1	B	581	GLY	4.8
1	B	786	MET	4.7
1	B	397	PHE	4.7
1	B	432	LEU	4.7
1	A	750	GLY	4.5
1	A	800	LEU	4.5
1	B	775	THR	4.5
1	D	953	PHE	4.5
1	A	785	SER	4.5
1	B	371	ILE	4.5
1	C	500	TYR	4.5
1	C	576	VAL	4.4
1	A	702	ILE	4.4
1	D	371	ILE	4.4
1	C	1213	VAL	4.3
1	D	631	SER	4.3
1	B	953	PHE	4.3
1	A	792	ALA	4.3
1	D	797	GLN	4.2
1	B	576	VAL	4.2
1	D	394	ASN	4.2
1	A	394	ASN	4.2
1	A	804	PHE	4.1
1	A	793	LEU	4.1
1	A	810	LEU	4.1
1	C	775	THR	4.0
1	A	784	ILE	4.0
1	B	370	VAL	4.0
1	A	812	LYS	4.0
1	B	395	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	815	ILE	3.9
1	D	987	ILE	3.9
1	D	369	ARG	3.9
1	C	367	ASN	3.9
1	B	654	VAL	3.9
1	D	988	ILE	3.9
1	D	581	GLY	3.9
1	A	807	VAL	3.9
1	C	813	HIS	3.9
1	D	500	TYR	3.9
1	A	653	VAL	3.8
1	A	575	ASP	3.8
1	D	804	PHE	3.8
1	B	647	ALA	3.8
1	D	575	ASP	3.8
1	A	953	PHE	3.7
1	C	812	LYS	3.7
1	C	1210	SER	3.7
1	B	502	GLY	3.7
1	B	648	PHE	3.7
1	C	803	VAL	3.6
1	A	419	PHE	3.6
1	A	779	ILE	3.6
1	C	784	ILE	3.6
1	B	414	ASP	3.6
1	D	551	GLY	3.6
1	B	804	PHE	3.5
1	C	792	ALA	3.5
1	D	647	ALA	3.5
1	B	557	ILE	3.5
1	A	698	VAL	3.5
1	D	786	MET	3.5
1	C	575	ASP	3.5
1	C	501	VAL	3.5
1	A	805	ASN	3.5
1	C	804	PHE	3.5
1	D	938	PRO	3.5
1	C	786	MET	3.5
1	B	658	LEU	3.5
1	B	787	LYS	3.4
1	A	415	LEU	3.4
1	C	578	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	562	GLU	3.4
1	C	652	GLY	3.4
1	C	805	ASN	3.4
1	D	978	GLY	3.4
1	D	811	GLU	3.4
1	B	606	LEU	3.4
1	D	633	ASN	3.3
1	B	789	ALA	3.3
1	B	472	ASP	3.3
1	B	418	GLU	3.3
1	B	796	TYR	3.3
1	A	367	ASN	3.3
1	C	953	PHE	3.3
1	D	768	ARG	3.3
1	B	984	ALA	3.3
1	D	983	GLY	3.2
1	C	702	ILE	3.2
1	D	1103	GLU	3.2
1	D	471	HIS	3.2
1	C	852	GLU	3.2
1	D	932	THR	3.2
1	B	803	VAL	3.2
1	B	556	GLN	3.2
1	D	472	ASP	3.2
1	B	791	ASP	3.1
1	B	811	GLU	3.1
1	B	653	VAL	3.1
1	B	417	ARG	3.1
1	D	559	SER	3.1
1	B	553	PRO	3.1
1	C	807	VAL	3.1
1	D	807	VAL	3.1
1	C	646	ALA	3.1
1	B	978	GLY	3.1
1	D	782	GLY	3.1
1	A	986	SER	3.1
1	A	991	PHE	3.1
1	A	370	VAL	3.1
1	D	576	VAL	3.1
1	D	981	VAL	3.1
1	A	1227	GLY	3.0
1	C	777	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	654	VAL	3.0
1	A	652	GLY	3.0
1	B	813	HIS	3.0
1	A	609	VAL	3.0
1	C	796	TYR	3.0
1	D	984	ALA	3.0
1	D	632	ASP	3.0
1	A	631	SER	3.0
1	A	987	ILE	3.0
1	B	649	ALA	3.0
1	B	981	VAL	3.0
1	C	432	LEU	3.0
1	D	611	PRO	3.0
1	D	809	GLU	3.0
1	C	653	VAL	3.0
1	D	367	ASN	3.0
1	A	576	VAL	2.9
1	D	831	LEU	2.9
1	D	557	ILE	2.9
1	D	556	GLN	2.9
1	B	801	GLU	2.9
1	B	436	LEU	2.9
1	A	646	ALA	2.9
1	A	501	VAL	2.9
1	C	787	LYS	2.9
1	A	581	GLY	2.9
1	B	543	LEU	2.9
1	C	831	LEU	2.9
1	C	417	ARG	2.8
1	D	1110	THR	2.8
1	C	986	SER	2.8
1	A	803	VAL	2.8
1	A	1213	VAL	2.8
1	D	769	GLY	2.8
1	C	987	ILE	2.8
1	D	812	LYS	2.8
1	D	775	THR	2.8
1	C	436	LEU	2.8
1	C	581	GLY	2.8
1	B	792	ALA	2.8
1	A	472	ASP	2.8
1	B	609	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	1025	ILE	2.8
1	D	396	ARG	2.8
1	D	858	PRO	2.8
1	A	658	LEU	2.8
1	D	1066	VAL	2.8
1	A	657	THR	2.8
1	D	642	LEU	2.8
1	B	1213	VAL	2.7
1	D	936	GLY	2.7
1	C	377	TYR	2.7
1	B	642	LEU	2.7
1	A	988	ILE	2.7
1	D	1025	ILE	2.7
1	B	555	SER	2.7
1	A	777	ALA	2.7
1	C	1216	VAL	2.7
1	B	987	ILE	2.7
1	A	701	MET	2.7
1	D	609	VAL	2.7
1	D	784	ILE	2.7
1	D	658	LEU	2.7
1	D	893	GLY	2.7
1	D	777	ALA	2.7
1	C	988	ILE	2.6
1	A	398	ARG	2.6
1	C	506	PHE	2.6
1	C	984	ALA	2.6
1	D	937	THR	2.6
1	C	793	LEU	2.6
1	B	795	ASP	2.6
1	D	934	PRO	2.6
1	A	506	PHE	2.6
1	A	606	LEU	2.6
1	C	373	LEU	2.6
1	A	794	ARG	2.6
1	A	1216	VAL	2.6
1	D	653	VAL	2.6
1	A	654	VAL	2.6
1	B	698	VAL	2.6
1	B	759	TYR	2.6
1	B	749	GLU	2.6
1	A	633	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	796	TYR	2.6
1	B	393	ASP	2.6
1	C	414	ASP	2.6
1	A	655	ALA	2.6
1	D	955	ALA	2.6
1	B	784	ILE	2.6
1	C	580	LEU	2.6
1	D	1213	VAL	2.5
1	C	950	LEU	2.5
1	D	415	LEU	2.5
1	D	649	ALA	2.5
1	A	578	TYR	2.5
1	D	416	ASP	2.5
1	A	373	LEU	2.5
1	B	1103	GLU	2.5
1	B	983	GLY	2.5
1	D	940	GLY	2.5
1	A	397	PHE	2.5
1	D	414	ASP	2.5
1	B	471	HIS	2.5
1	B	798	GLY	2.5
1	C	983	GLY	2.5
1	D	1009	LEU	2.5
1	D	553	PRO	2.5
1	B	503	GLN	2.5
1	D	791	ASP	2.5
1	A	650	GLY	2.5
1	D	634	ARG	2.4
1	A	414	ASP	2.4
1	D	418	GLU	2.4
1	B	782	GLY	2.4
1	D	796	TYR	2.4
1	A	768	ARG	2.4
1	A	789	ALA	2.4
1	B	701	MET	2.4
1	D	805	ASN	2.4
1	A	950	LEU	2.4
1	C	1007	LEU	2.4
1	D	801	GLU	2.4
1	B	473	LYS	2.4
1	C	609	VAL	2.4
1	C	776	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	369	ARG	2.3
1	C	503	GLN	2.3
1	D	928	GLN	2.3
1	D	630	GLY	2.3
1	D	935	ASP	2.3
1	B	988	ILE	2.3
1	D	1065	ILE	2.3
1	A	740	LEU	2.3
1	A	799	GLN	2.3
1	B	954	ALA	2.3
1	C	657	THR	2.3
1	C	1060	ILE	2.3
1	D	776	GLU	2.3
1	A	608	ALA	2.3
1	B	420	LYS	2.3
1	A	1023	GLY	2.3
1	B	778	LEU	2.3
1	D	473	LYS	2.3
1	D	975	ALA	2.3
1	A	775	THR	2.3
1	B	783	ASP	2.3
1	D	1060	ILE	2.3
1	C	789	ALA	2.3
1	B	559	SER	2.3
1	B	558	PHE	2.2
1	C	783	ASP	2.2
1	D	558	PHE	2.2
1	C	476	VAL	2.2
1	C	981	VAL	2.2
1	A	503	GLN	2.2
1	B	797	GLN	2.2
1	D	951	SER	2.2
1	D	973	TRP	2.2
1	A	695	CYS	2.2
1	C	937	THR	2.2
1	D	991	PHE	2.2
1	B	676	VAL	2.2
1	A	1212	LYS	2.2
1	D	954	ALA	2.2
1	C	606	LEU	2.2
1	B	1225	ALA	2.2
1	A	500	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	863	VAL	2.2
1	D	920	THR	2.2
1	A	611	PRO	2.2
1	B	938	PRO	2.2
1	B	578	TYR	2.2
1	C	759	TYR	2.2
1	B	396	ARG	2.2
1	B	928	GLN	2.1
1	A	831	LEU	2.1
1	B	415	LEU	2.1
1	B	812	LYS	2.1
1	A	495	PHE	2.1
1	C	1083	ARG	2.1
1	D	648	PHE	2.1
1	A	649	ALA	2.1
1	D	555	SER	2.1
1	B	916	VAL	2.1
1	C	590	PHE	2.1
1	A	647	ALA	2.1
1	B	800	LEU	2.1
1	B	1035	GLY	2.1
1	C	642	LEU	2.1
1	A	951	SER	2.1
1	A	505	ARG	2.1
1	C	749	GLU	2.1
1	B	706	ILE	2.1
1	A	432	LEU	2.1
1	A	1029	LEU	2.1
1	D	606	LEU	2.1
1	C	1023	GLY	2.1
1	B	808	ARG	2.0
1	D	783	ASP	2.0
1	D	1007	LEU	2.0
1	A	909	THR	2.0
1	A	558	PHE	2.0
1	B	554	TYR	2.0
1	B	858	PRO	2.0
1	C	411	THR	2.0
1	D	789	ALA	2.0
1	B	940	GLY	2.0
1	C	808	ARG	2.0
1	D	627	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	935	ASP	2.0
1	B	836	ASP	2.0
1	A	377	TYR	2.0
1	A	607	GLU	2.0
1	C	920	THR	2.0
1	C	1035	GLY	2.0
1	D	956	VAL	2.0

6.2　Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3　Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4　Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TD9	B	2001	34/34	0.95	0.18	20,32,69,73	0
3	MG	A	2002	1/1	0.95	0.16	25,25,25,25	0
3	MG	B	2002	1/1	0.95	0.12	28,28,28,28	0
2	TD9	A	2001	34/34	0.96	0.17	24,32,63,65	0
2	TD9	C	2001	34/34	0.96	0.17	23,30,57,58	0
4	CA	B	2003	1/1	0.96	0.05	43,43,43,43	0
4	CA	D	2003	1/1	0.96	0.06	41,41,41,41	0
2	TD9	D	2001	34/34	0.97	0.17	18,29,63,65	0
3	MG	D	2002	1/1	0.98	0.11	24,24,24,24	0
4	CA	A	2003	1/1	0.98	0.05	38,38,38,38	0
4	CA	C	2003	1/1	0.99	0.04	38,38,38,38	0
3	MG	C	2002	1/1	0.99	0.16	22,22,22,22	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.
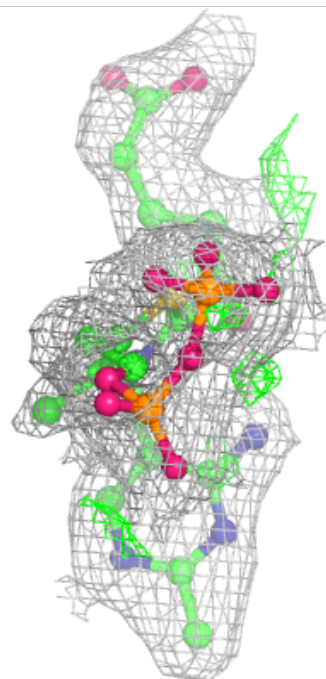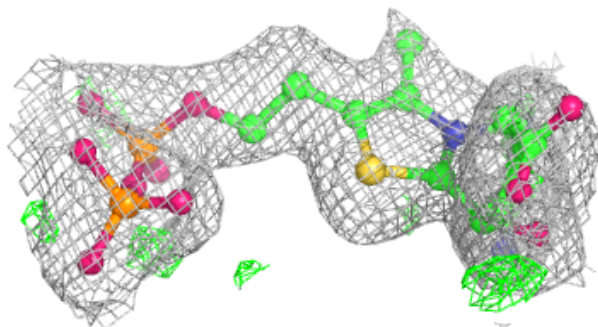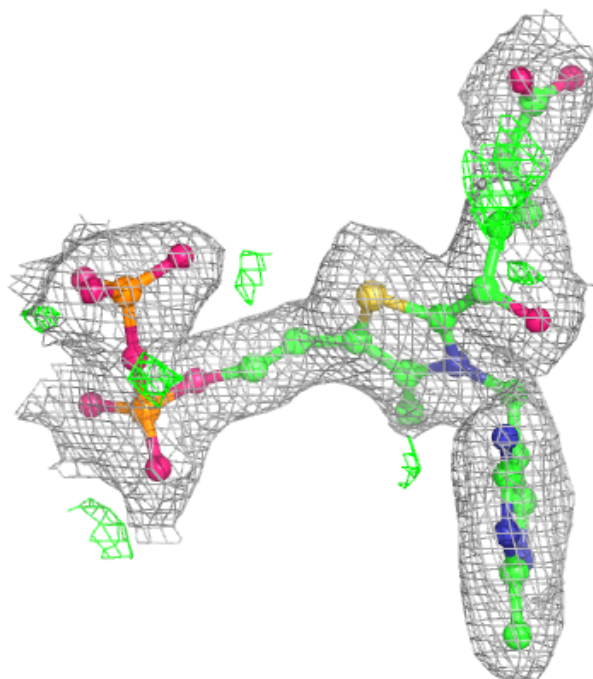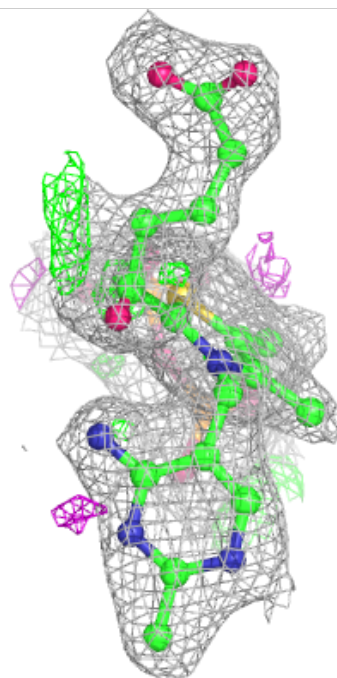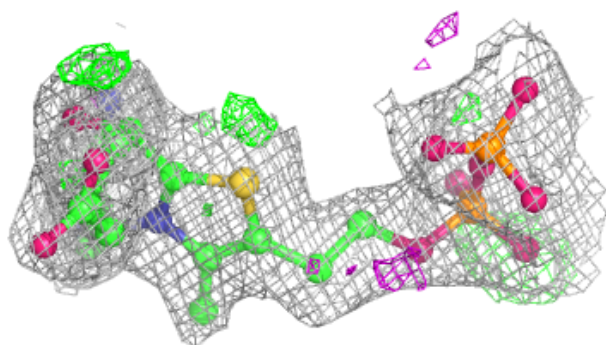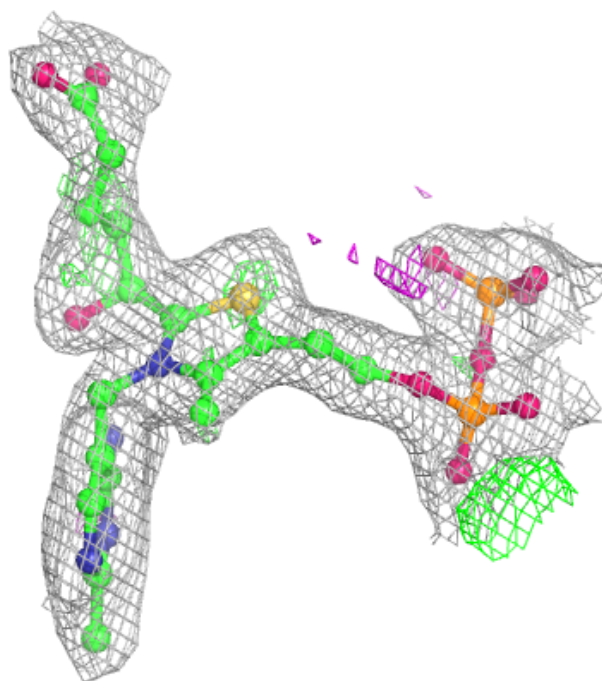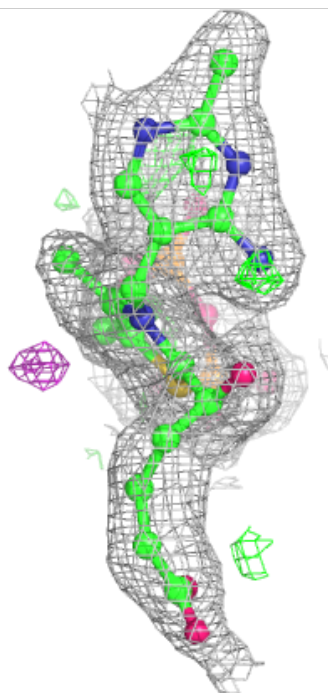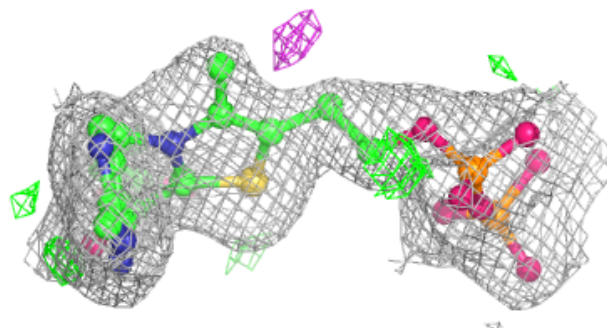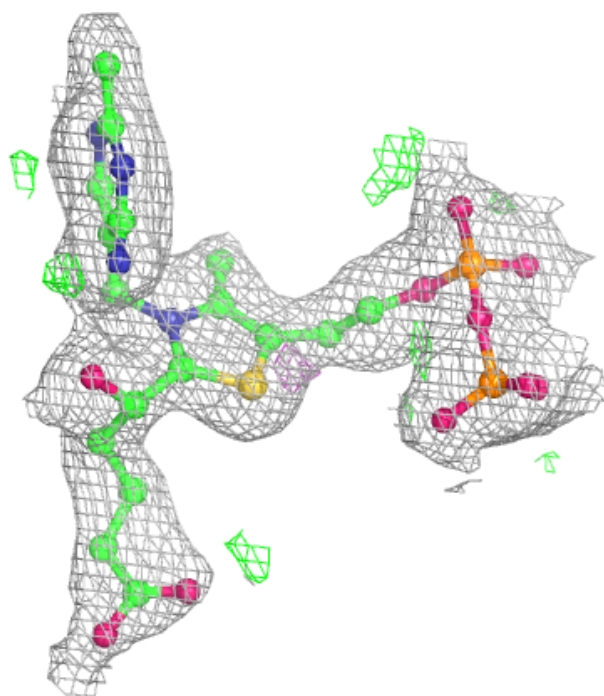
WORLDWIDE
wwPDB
PROTEIN DATA BANK

Electron density around TD9 B 2001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
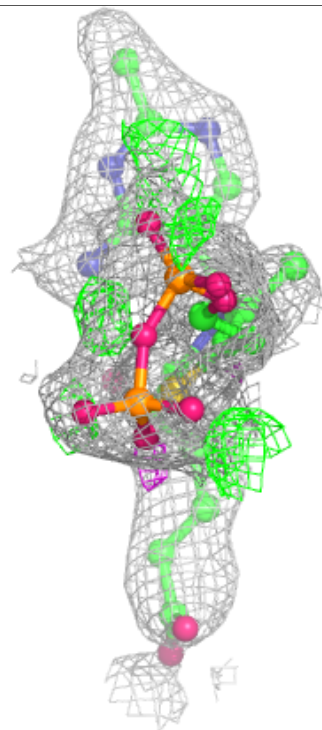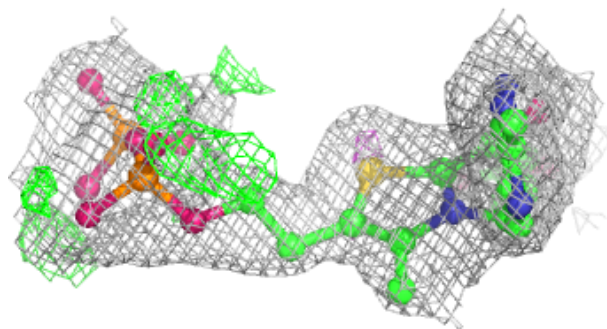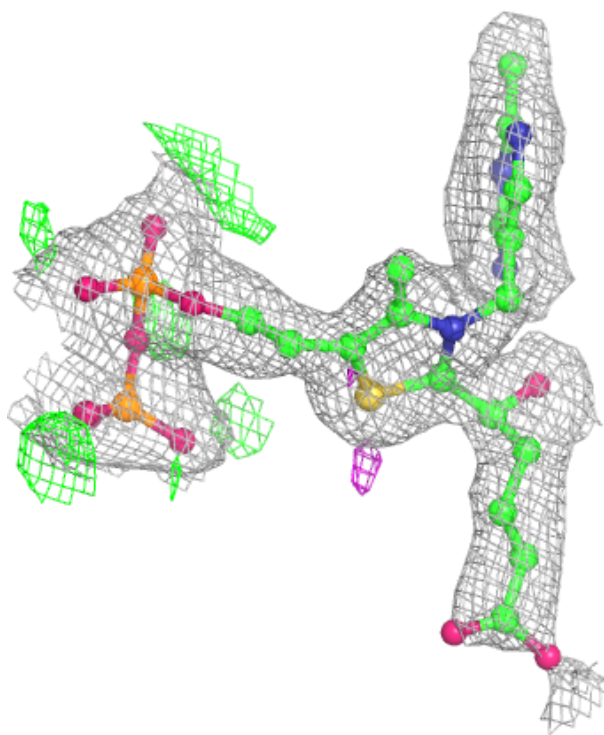
Electron density around TD9 A 2001:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around TD9 C 2001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around TD9 D 2001:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers (i)

There are no such residues in this entry.